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OPTIMIZATION AND DESIGN OF 2D HONEYCOMB LATTICE PHOTONIC CRYSTAL MODULATED BY LIQUID CRYSTALS

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Photonic crystals (PCs) with infiltrating liquid crystals (LCs) have many potential applications because of their ability to continuously modulate the band-gaps. Using the plane-wave expansion method (PWM), we simulate the band-gap distribution of 2D honeycomb lattice PC with different pillar structures (circle, hexagonal and square pillar) and with different filling ratios, considering both when the LC is used as filling pillar material and semiconductors (Si, Ge) are used in the substrate, and when the semiconductors (Si, Ge) are pillar material and the LC is the substrate. Results show that unlike LC-based triangle lattice PC, optimized honeycomb lattice PC has the ability to generate absolute photonic band-gaps for fabricating optical switches. We provide optimization parameters for LC infiltrating honeycomb lattice PC structure based on simulation results and analysis.

Keywords: Photonic crystal; liquid crystal; photonic band-gaps; plane-wave expansion method; optical switch.

1. Introduction

Photonic crystal (PC)[1,2] is a kind of optical nanostructure with materials of different dielectric constants in the periodic arrangement. This feature is what allows PC to have photonic band-gaps, and therefore the ability to forbid photons of a frequency within a forbidden band to spread in the crystal. Due to the existence of PBGs, PCs have been considered having many potential applications such as light emitting diode (LED)[3] filters,[4] humidity sensor,[5] etc. However, PBG distribution

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cannot be changed once the structure of PC is determined, which greatly restricts the development of PC based devices. In order to overcome this limitation, the PCs infiltrated with liquid crystals (LCs) are proposed,[6−10] whose PBG distribution could be adjusted if an external electrical field is applied to the PC to adjust the effective refractive index of the LCs. Therefore, this finding led to widespread interest in the development of many LC-based PC devices such as optical attenuators,[9] filters,[11] fiber,[12] field-sensitive polarizers,[13] optical switches,[14] etc. But, the triangular lattice PC, filled with LC in the air pillar, does not generate absolute PBG when semiconductors Si and Ge are substrate materials that have been proposed.[15] It is important, however, to obtain better PBGs of PC.

To continue the search for a better PBG structure, we study the honeycomb lattice PC[16−18] composed of LC. 2D honeycomb lattice structure is a kind of 2D periodic array, of mutually parallel and axially infinitely extended pillars, formed by extracting a certain number of pillars in triangular lattice. Honeycomb lattice is a kind of fullerene stable nanostructure for the applications including PC fiber[19,20] PC laser[21] and so on. The results show that absolute PBGs appear if the refractive index of the LC equals its ordinary refractive index value, applied with enough external voltage, while PBGs are absent when the extraordinary refractive index occurs, without the driving voltage. Potentially, therefore, electrically controlled optical switch devices based on tunable PC can be fabricated. Compared to PC optical switch with insertion of line defect into the crystal for defective modes migrating,[8,14] this kind of switch, with the benefit of PBG migration, is simpler and easier to realize.

In order to optimize the properties of PC devices with PBG migration, it is necessary to optimize the design of structure for generating the PBG. In this paper, we simulated the PBG distribution of 2D honeycomb lattice PCs composed of LC and two semiconductor materials, Si and Ge respectively, and analyzed and optimized a series of PBG distributions considering different structural parameters including pillar shapes, packing ratio, refractive index of LC, and polarization dependence. The optimized structure identified in our study should provide better guidance for the implementation of LC based PC devices.

2. Numerical Simulation Methods

In this paper, we use the plane wave expansion method (PWM),[22] the earliest proposed and the most widely used method for calculating and analyzing crystal structure and band-gaps of PCs, to simulate the PBGs of 2D honeycomb lattice PCs. The basic idea is to expand electromagnetic waves in the form of plane waves, to transform Maxwell equations into an eigenequation and solve the eigenvalues to obtain PBG.

In our model, the value of PBG is determined by the transmission electromagnetic field, while redistribution of the PBG occurs through rotating the direction of the LC droplets. Electromagnetic wave equations within 2D plane can be

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expressed as

$$\nabla \times \left[\frac{1}{\varepsilon(\mathbf{r})}\nabla \times \mathbf{H}(\mathbf{r})\right] = \left(\frac{\omega}{c}\right)^2 \mathbf{H}(\mathbf{r})\,, \tag{1}$$

$$\frac{1}{\varepsilon(\mathbf{r})}\nabla \times \nabla \times E(\mathbf{r}) = \left(\frac{\omega}{\mathbf{r}}\right)^2 E(\mathbf{r})\,, \tag{2}$$

where the dielectric tensor $\varepsilon(\mathbf{r}) = \varepsilon(\mathbf{r} + a)$ is a periodic function with respect to lattice vector, which is generated by primitive translation, and a is lattice constant. $E(\mathbf{r})$ is expanded to a series of plane waves, and Eqs. (1) and (2) are transformed into a system of linear equations. By solving the above equations, we can obtain the frequency modes related to the wave vector.

Due to their birefringence characteristic, LCs usually have two dielectric indices, the ordinary dielectric index ε^o, and extraordinary dielectric index ε^e. In 2D PCs, electromagnetic waves travel in the form of two polarization modes, namely TE and TM. We assume that the optical axis of LC is within the x–z plane. The incident light is along the z-direction and the electric field is parallel to the direction of x.

In a 2D plane, the components of the dielectric tensor of nematic LCs are presented as

$$\varepsilon_{xx}(\mathbf{r}) = \varepsilon^o(\mathbf{r})\sin^2\phi + \varepsilon^e(\mathbf{r})\cos^2\phi\,, \tag{3}$$

$$\varepsilon_{zz}(\mathbf{r}) = \varepsilon^o(\mathbf{r})\cos^2\phi + \varepsilon^e(\mathbf{r})\sin^2\phi\,, \tag{4}$$

$$\varepsilon_{xz}(\mathbf{r}) = \varepsilon_{xz}(\mathbf{r}) = [\varepsilon^e(\mathbf{r}) - \varepsilon^o(\mathbf{r})]\cos\phi\sin\phi\,, \tag{5}$$

where ϕ is the rotation angle of the LC director. And $n = (\cos\phi, \sin\phi)$ is the LC director, as shown in Fig. 1. It is obvious that when a light wave with electric fields is perpendicular to the LC director, i.e. $\phi = 0°$, the LCs exhibit ordinary index characteristic, while if the wave with electric fields is parallel to the LC director, i.e. $\phi = 90°$, the LCs have extraordinary refractive index. In addition, according to the description of Li and others,[23–25] the z-direction of propagation indicates the direction of the energy gap.

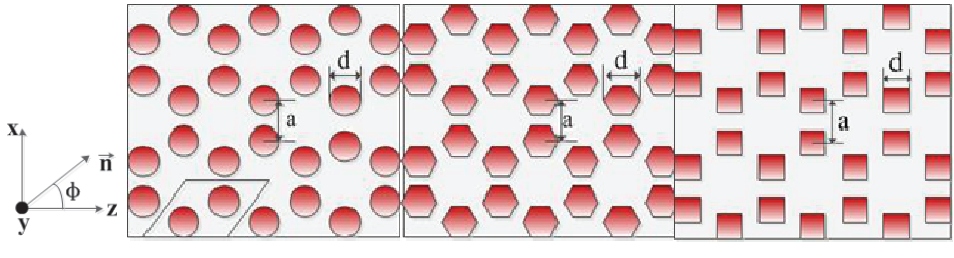

Fig. 1. (Color online) Model of honeycomb lattice PCs with circular, square, hexagon pillar structure (the left inset indicates the director of a liquid crystal).

In our simulation, the 2D Honeycomb lattice PC was filled with phenylacetylene LC[14,26] and semiconductor mediums Si ($n_{\mathrm{Si}} = 3.44$) and Ge ($n_{\mathrm{Ge}} = 4$) respectively. Compared to 5CB LC ($n_o = 1.522$ and $n_e = 1.702$),[9] the phenylacetylene LC ($n_o = 1.59$ and $n_e = 2.223$) has a broader of refractive index range, thus resulting in better PBG distribution. In the structure of 2D honeycomb lattice, the maximum band-gap width of the PC is very stable, and other parameters such as the pillar shapes and angle of rotation have little effect on the PBG. Figure 1 shows the 2D honeycomb lattice PC with three pillar structures. a is the center-to-center distance of two adjacent pillars, i.e. the lattice constant, (default value is 1 μm); and d is the diameter of the pillar.

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3. Simulation and Analysis of PCs with LC as Substrate Material

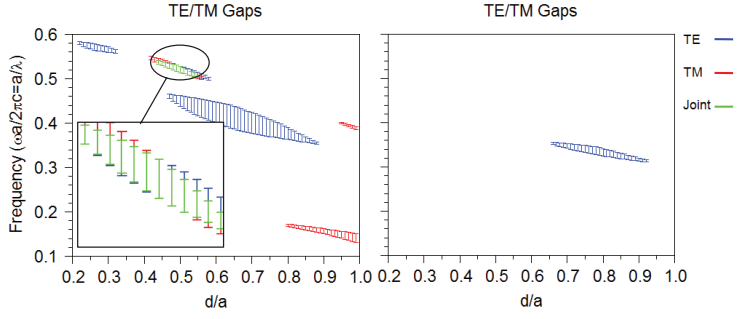
The PWM is used to calculate the TE and TM gaps of the PCs with LC as substrate material varying with the diameter, d, from $0.01a$ to $0.99a$ at the step-size of $0.01a$, and that the rotation angles of the LC director are $\phi = 0°(n^o_{\mathrm{LC}} = 1.59)$ and $\phi = 90°(n^e_{\mathrm{LC}} = 2.223)$. The medium pillars are made from Si or Ge, and the pillar shapes are circle, hexagon, and square respectively. We do not take the dispersion of the constitutive materials into account in the ideal model (the Rsoft software was used for PC simulation).

3.1. *PCs with Si filling dielectric pillar*

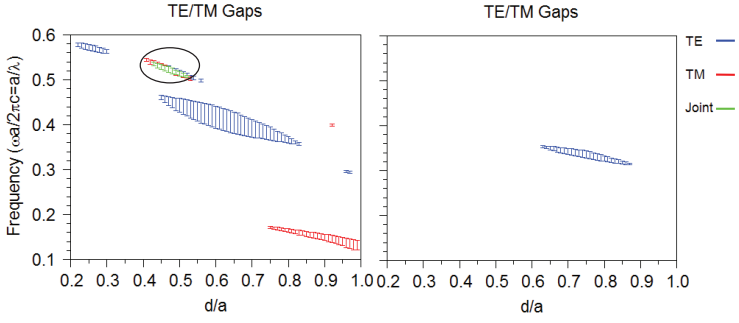
The results are illustrated in Fig. 2. As can be seen, when the dielectric pillar is made from Si, band-gaps in the two polarization modes overlap with each other in all cases of $\phi = 0°$, indicating the presence of absolute PBGs. By contrast, the absolute PBGs are absent when $\phi = 90°$. The result confirms PC based optical switches within this frequency range can be realized, because the photons within this frequency range move in and out of the energy gap, for the adjustability of honeycomb lattice PC filled with LC. Furthermore by adjusting the lattice constant (a) appropriately, very simple optical switches, for different wavelengths of light, can be achieved.

For the cylindrical circular structure, absolute PBGs exist when d/a is within the range of 0.44–0.55. The corresponding results are listed in Table 1. Furthermore, the largest band-gap frequency range ($\Delta_{\max} = 0.5279 - 0.5136 = 0.0143$), is located at the position of $d = 0.5a$. Thus, the frequency range of optical switches can be set at $\omega a/(2\pi c) = 0.5279 \sim 0.5136$. Depending on the d/a values, the frequency range ($0.5406 \sim 0.5029$) of light switches can be realized.

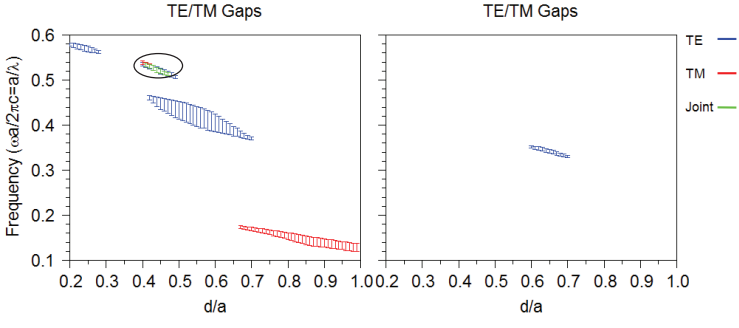
Table 1 gives the band-gap parameters for all three versions of the 2D honeycomb lattice PC. For the lattices with hexagon and square pillars, we can see that the frequency range of the absolute PBGs becomes smaller, but overall change is not obvious. This tells us that pillar shape has little effect on the band-gap of 2D honeycomb lattice PCs.



(a) Circle pillar (left: $\phi = 0°$, right: $\phi = 90°$).



(b) Hexagon pillar (left: $\phi = 0°$, right: $\phi = 90°$).



(c) Square pillar (left: $\phi = 0°$, right: $\phi = 90°$).

Fig. 2. (Color online) TE/TM band-gap for Si dielectric pillar when d/a changes continuously.

Table 1. The band-gap characteristic of 2D honeycomb lattice PC modulated by LC (dielectric Si filling the pillar).

Pillar shape	The range of d/a	The range of band-gap frequency ($\omega a/2\pi c$)	Diameter (d)	$\Delta_{\max}$
Circle	0.44–0.55	0.5406–0.5029	$d = 0.5a$	0.0143
Hexagon	0.43–0.52	0.5387–0.5046	$d = 0.47a$	0.0134
Square	0.41–0.47	0.5370–0.5104	$d = 0.43a$	0.0106

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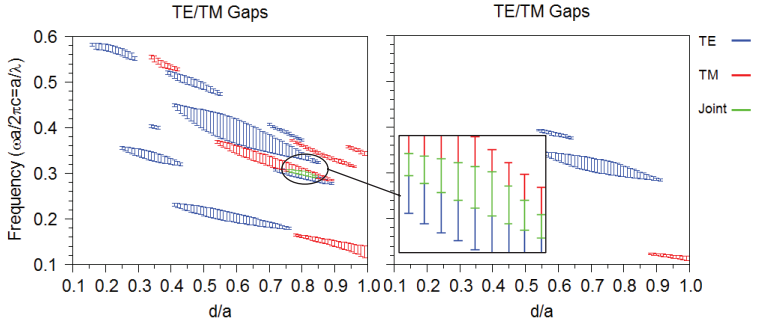
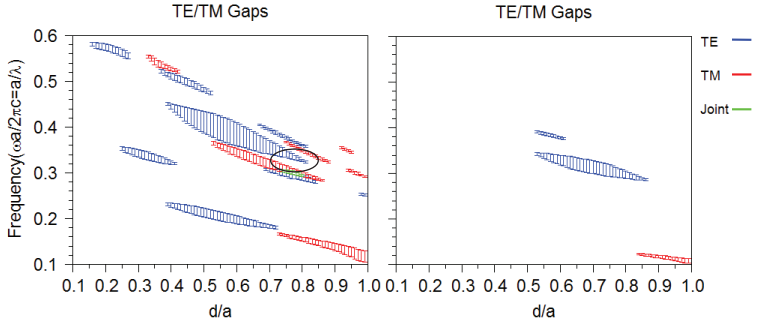
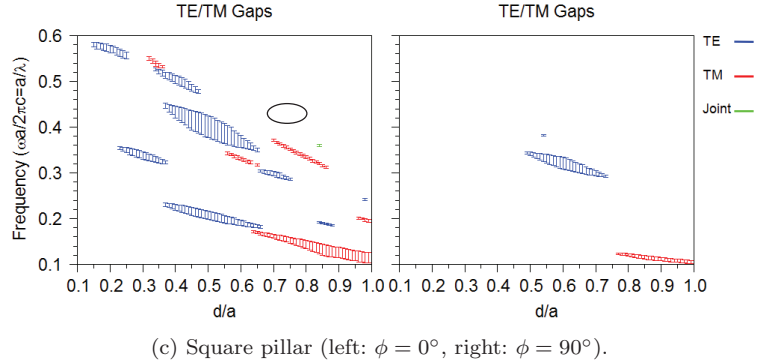


(a) Circle pillar (left: $\phi = 0°$, right: $\phi = 90°$).



(b) Hexagon pillar (left: $\phi = 0°$, right: $\phi = 90°$).



(c) Square pillar (left: $\phi = 0°$, right: $\phi = 90°$).

Fig. 3. (Color online) TE/TM band-gap for Ge dielectric pillar when d/a changes continuously.

3.2. *PCs with Ge filling dielectric pillar*

From Fig. 3(a), we can see that when the dielectric cylinder is Ge, $\phi = 0°$, and d/a is in the range of $0.76 \sim 0.84$, absolute PBGs exist, the numerical results are listed in Table 2. The largest band-gap frequency is $\Delta_{\max} = 0.3045 - 0.2952 = 0.0093$ at the position of $d = 0.81a$. But for $\phi = 90°$, for the same packing ratio, the band-gap in TE mode is produced in the same frequency range. Thus, this structure can be used to realize switching devices for TM polarized light within the normalized frequency

Table 2. The absolute band-gap characteristic of 2D honeycomb lattice PC modulated by LC (dielectric Ge filling the pillar).

Pillar shape	The range of d/a	The range of band-gap frequency ($\omega a/2\pi c$)	Diameter (d)	$\Delta_{\max}$
Circle	0.76–0.84	0.3084–0.2905	$d = 0.81a$	0.0093
Hexagon	0.74–0.8	0.3072–0.2917	$d = 0.77a$	0.0078

from 0.3084 to 0.2905. For example, unpolarized light of frequency $\omega a/(2\pi c) = 0.3$ cannot be transmitted if $\phi = 0°$ at the position $d = 0.81a$. By contrast, only TM-polarized light will be transmitted if $\phi = 90°$. Similarly, in the case of the hexagonal pillar, the band-gap range is shown in Table 2, and even little change occurs compared to the cylindrical structure. In addition, the available band-gap frequency for TM polarized light switch is at $\omega a/(2\pi c) = 0.3072 \sim 0.2917$.

Regarding the square pillars, the TE/TM band-gap distribution is shown in Fig. 3(c). The absolute PBG is only at $d/a = 0.84$, but it is a "pseudo absolute photonic band-gap", which does not exist actually because of the shortage of wave numbers.

4. Simulation and Analysis of PCs with LC as Pillar Material

PCs with air hole pillars are easy to manufacture and integrate. The simulation result for the 2D honeycomb lattice PCs with LC-filled air hole pillars are shown as follows.

4.1. *PCs with Si as substrate material*

The numerical results demonstrate that when the pillar shapes are circle and hexagon, there are no absolute PBGs for $\phi = 0°$ nor for $\phi = 90°$. Only under the condition of the square pillar does, the small absolute PBGs appear at $d = 0.98a$ and $d = 0.99a$, as shown in Fig. 4. The range of band-gap frequency is

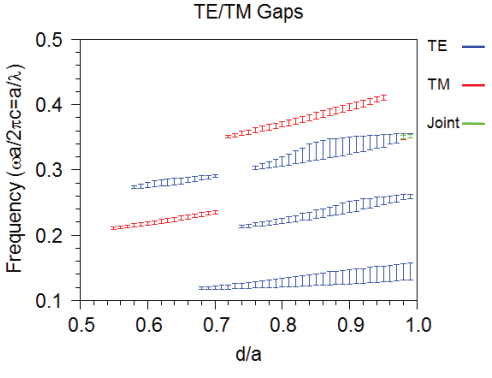


Fig. 4. (Color online) TE/TM band-gap for Si as substrate material when d/a changes continuously (square pillar and $\phi = 0°$).

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Table 3. The absolute band-gap characteristic of 2D honeycomb lattice PC modulated by LC (Ge as substrate material).

Pillar shape	The range of d/a	The range of band-gap frequency ($\omega a/2\pi c$)	Diameter (d)	$\Delta_{\max}$
Circle	0.94–0.99	0.3084–0.2810	$d = 0.98a$	0.0134
Hexagon	0.88–0.96	0.3129–0.2763	$d = 0.95a$	0.0189
Square	0.76–0.9	0.3094–0.2614	$d = 0.82a$	0.0132

$\Delta_{0.98} = 0.3530 - 0.3478 = 0.0052$ and $\Delta_{0.99} = 0.3546 - 0.3492 = 0.0054$, respectively. Absolute PBGs are absent when $\phi = 90°$. Therefore, optical switches can be achieved for the normalized frequency of 0.3546–0.3478 when substrate material is Si.

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4.2. *PCs with Ge as substrate material*

Figure 5 shows the TE/TM band-gaps of the PCs modulated by LC with Ge as substrate. When pillars are cylinders (Fig. 5(a)), there are absolute band-gaps when $\phi = 0°$ and d/a is from 0.94 to 0.99. Similarly they are absent when $\phi = 90°$. The largest band-gap ($\Delta_{\max} = 0.3038 - 0.2904 = 0.0134$) lies in the position of $d = 0.98a$. Therefore, optical switching can be realized within the normalized frequency range of $0.3038 \sim 0.2904$. Figure 5(a) also shows that depending on the different packing ratios, the optical switches for normalized frequency range of $0.3084 \sim 0.2810$ are made from the whole band-gap structure. The results are similar for the cases of hexagon and square pillars shown in Figs. 5(b) and 5(c), where it can be seen that the PBG distributions change slightly. The calculated results are listed in Table 3.

Table 4 gives the available frequency range for optical switches of 2D honeycomb lattice PC modulated by LC according to different packing ratios. The maximum band-gap width is 0.048 (d/a is from 0.79 to 0.9), when LC is the square pillar material and Ge is used as substrate material. Furthermore, when LC is used as the substrate, a larger band-gap is produced by PCs with Si pillars and there is a wider frequency range for the optical switch. PCs with Ge-filled dielectric pillars can be used to develop switches for the specific frequency of TM polarized light. For the case of LC filling pillars, when there are absolute PBGs, the packing

Table 4. The available frequency of 2D honeycomb lattice PC modulated by LC on the different conditions.

		Pillar shape		
	Material	Circle ($\omega a/2\pi c$)	Hexagon ($\omega a/2\pi c$)	Square ($\omega a/2\pi c$)
LC as substrate material	Si as pillar material	0.5406–0.5029	0.5387–0.5046	0.5370–0.5104
	Ge as pillar material	0.3084–0.2905 (TM)	0.3072–0.2917 (TM)	null
LC as pillar material	Si as substrate material	null	null	0.3546–0.3478
	Ge as substrate material	0.3084–0.2810	0.3129–0.2763	0.3094–0.2614

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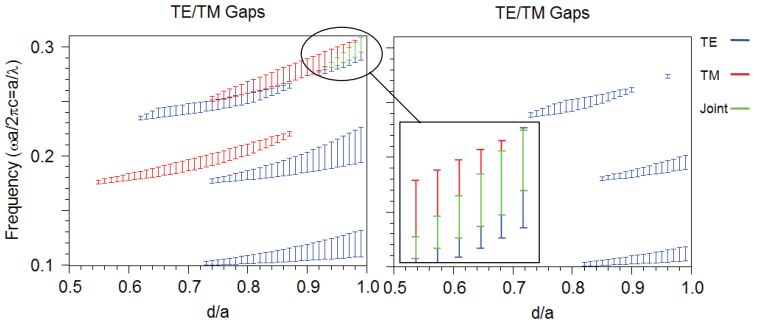
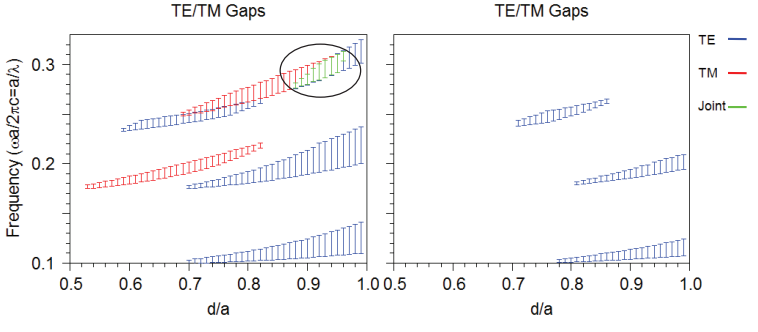
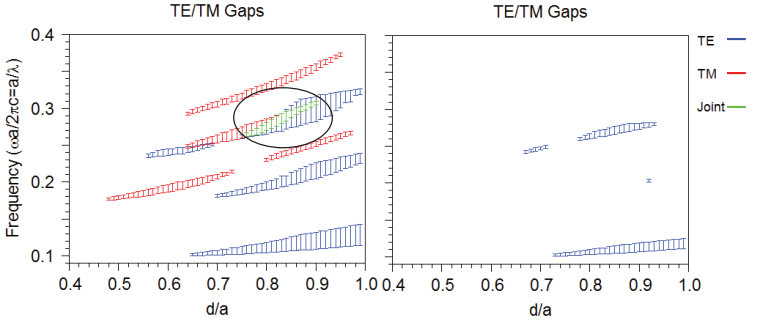


(a) Circle pillar (left: $\phi = 0°$, right: $\phi = 90°$).



(b) Hexagon pillar (left: $\phi = 0°$, right: $\phi = 90°$).



(c) Square pillar (left: $\phi = 0°$, right: $\phi = 90°$).

Fig. 5. (Color online) TE/TM band-gap for Ge as substrate material when d/a changes continuously.

ratios are bigger. Thus, it is better in the connectivity, easier to produce in the process.

4.3. *PBG variation with the director of LC*

A comparison of Tables 1–3 shows that when LC is used as pillar material, and Ge as substrate material, the absolute PBG is maximum at the position of $d = 0.95a$.

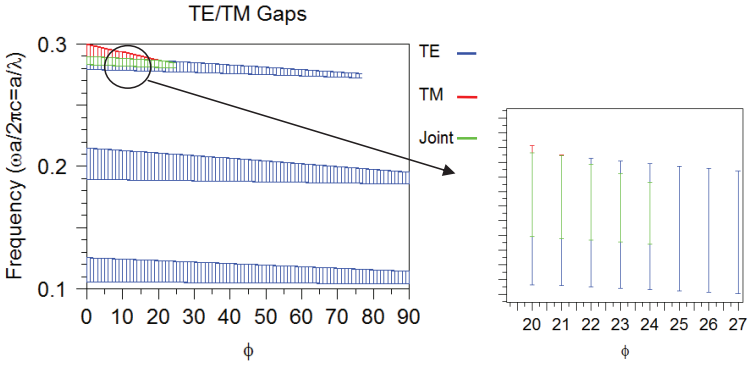


Fig. 6. The PBG variation with the director of LC while $d = 0.95a$.

Consequently, we simulated the PBG of this PC variation with its corresponding LC director and the result is shown as Fig. 6. When the LC director is changed from 24° to 25°, the absolute PBG disappears, meaning, the switch is open. This makes it easy to determine the turn-on/off voltage. Although for the different structures, materials and packing ratio, PCs will have the different turn-on/off voltages for switches, it is still relatively easy to find this voltage by the rotated angle of LC director.

5. Conclusion

Our work shows that tunable PBGs in 2D LC modulated PCs are achievable. We used the PWM to calculate band-gaps of 2D honeycomb lattice PC modulated by LC, for the conditions of LC as substrate and pillar material respectively, and analyzed the influence of pillar shape and, packing ratio on the band-gap. The simulated results demonstrate that pillar shape has influence on the existence of absolute PBGs. Therefore, all we need for PBG migration in these structures is to control the refractive index of the LC with the external electrical field, and switches for a certain frequency range can be produced. Furthermore, switches for different wavelengths can be realized by adjusting different lattice constants. These finding provide theoretical guidance for further application of PC devices with LC modulation.

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